

chain nodes:

10

ring nodes:

1 2 3 4 5 6 7 8 9 12 13 14

chain bonds:

1-10

ring bonds:

1-2 1-6 2-3 2-7 3-4 3-9 4-5 5-6 7-8 7-12 8-9 12-13 13-14

exact/norm bonds:

1-2 1-6 1-10 2-3 2-7 3-4 3-9 4-5 5-6 7-8 7-12 8-9 12-13 13-14

G1:0,S

G2:C,N

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLAS\$12:Atom 13:Atom 14:Atom

### => d his

# (FILE 'HOME' ENTERED AT 16:17:21 ON 02 APR 2007)

	FILE	'REGISTRY'	ENTERED	AT 16:20	:02 ON	02 APR	2007							
L1	STRUCTURE UPLOADED													
L2	50 S L1													
L3	STRUCTURE UPLOADED													
L4		50 S L3												
L5	STRUCTURE UPLOADED													
L6		23 S L5												
L7		462 S L5	SSS FUL											
L8		445 S L7	AND CAPI	LUS/LC										
L9		17 S L7	NOT L8											

=> d 17

ANSWER 17 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN 300394-00-7 REGISTRY Entered STN: 30 Oct 2000 L9

RN

ED

CN 3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-3-[2-(4-methoxyphenyl)-2-oxoethyl]-4-oxo- (9CI) (CA INDEX NAME)

C21 H20 N4 O3 MF

Chemical Library SR

Supplier: Interbioscreen Ltd.

LC STN Files: CHEMCATS

ANSWER 16 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN 304869-03-2 REGISTRY Entered STN: 29 Nov 2000 L9

RN

ED

3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-3-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX CN NAME)

MF C20 H18 N4 O2

Chemical Library SR

Supplier: Interbioscreen Ltd.

STN Files: CHEMCATS LC

ANSWER 15 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN L9

RN

ED

304872-67-1 REGISTRY
Entered STN: 29 Nov 2000
3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, CN 4,6,7,8,9,10-hexahydro-3-[2-(4-nitrophenyl)-2-oxoethyl]-4-oxo- (9CI) (CA INDEX NAME)

C20 H17 N5 O4 MF

Chemical Library SR

Supplier: Interbioscreen Ltd.

STN Files: LC CHEMCATS

ANSWER 14 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN 305865-14-9 REGISTRY Entered STN: 01 Dec 2000 L9

RN

ED

3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 3-[(2-chlorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

C19 H17 Cl N4 O MF

SR Chemical Library

Supplier: Interbioscreen Ltd.

STN Files: CHEMCATS LC

$$N$$
 $N$ 
 $C1$ 
 $N$ 
 $CH_2$ 

ANSWER 13 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN L9

RN

327097-75-6 REGISTRY Entered STN: 14 Mar 2001 ED

3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, CN 3-[2-(4-chlorophenyl)-2-oxoethyl]-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

MF C20 H17 C1 N4 O2

Chemical Library SR

Supplier: Interbioscreen Ltd.

STN Files: CHEMCATS LC

$$\begin{array}{c|c}
CN & O & C1 \\
\hline
N & CH_2 - C & C1
\end{array}$$

LC

STN Files: CHEMCATS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Supplier: ChemBridge Corporation

L9 ANSWER 11 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN

RN 352555-04-5 REGISTRY

ED Entered STN: 24 Aug 2001

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 3-[(2-chlorophenyl)methyl]-3,4,6,7,8,9-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

MF C18 H15 C1 N4 O

SR Chemical Library

Supplier: Interbioscreen Ltd.

LC STN Files: CHEMCATS

$$N$$
 $N$ 
 $C1$ 
 $N$ 
 $CH_2$ 

ANSWER 10 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN 352555-05-6 REGISTRY Entered STN: 24 Aug 2001 L9

RN

ED

Pyrimido[4,5-b]indolizine-10-carbonitrile, 3-[2-(4-bromophenyl)-2oxoethyl]-3,4,6,7,8,9-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

MF C19 H15 Br N4 O2

Chemical Library SR

Supplier: Interbioscreen Ltd.

STN Files: CHEMCATS LC

L9 ANSWER 9 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN

RN 371927-57-0 REGISTRY

ED Entered STN: 27 Nov 2001

CN Pyrimido[4,5-b]indolizine-3(4H)-acetic acid, 10-cyano-6,7,8,9-tetrahydro-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

MF C14 H14 N4 O3

SR Chemical Library

Supplier: Interbioscreen Ltd.

LC STN Files: CHEMCATS

L9 ANSWER 8 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN

RN 371931-51-0 REGISTRY

ED Entered STN: 27 Nov 2001

CN 3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 3-[(4-chlorophenyl)acetyl]-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

MF C20 H17 C1 N4 O2

SR Chemical Library
Supplier: Ambinter

L9 ANSWER 7 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN

RN 413610-74-9 REGISTRY

ED Entered STN: 12 May 2002

CN 3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-3-acetic acid,

11-cyano-4,6,7,8,9,10-hexahydro-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)

MF C16 H18 N4 O3

SR Chemical Library

Supplier: ChemBridge Corporation

SR

ANSWER 6 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN 414904-55-5 REGISTRY Entered STN: 13 May 2002 L9

RN

ED

3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, CN 3-[2-(4-bromophenyl)-2-oxoethyl]-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

C20 H17 Br N4 O2 MF

Chemical Library

Supplier: ChemBridge Corporation

ANSWER 5 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN 414907-66-7 REGISTRY Entered STN: 13 May 2002

RN

ΕD

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 3,4,6,7,8,9-hexahydro-4-oxo-3-(2-oxo-2-phenylethyl) - (9CI) (CA INDEX NAME)

MF C19 H16 N4 O2

Chemical Library SR

Supplier: ChemBridge Corporation

STN Files: CHEMCATS LC

$$\begin{array}{c|c}
CN & O \\
N & CH_2-C-Ph
\end{array}$$

ANSWER 4 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN 415685-91-5 REGISTRY Entered STN: 14 May 2002 L9

RN

ED

3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-3-acetic acid, 11-cyano-4,6,7,8,9,10-hexahydro-4-oxo-, methyl ester (9CI) CN (CA INDEX NAME)

MF C15 H16 N4 O3

SR Chemical Library

Supplier: ChemBridge Corporation

LC STN Files: CHEMCATS

L9 ANSWER 3 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN

RN 425397-88-2 REGISTRY

ED Entered STN: 04 Jun 2002

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 3-[(4-chlorophenyl)methyl]-3,4,6,7,8,9-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

MF C18 H15 C1 N4 O

SR Chemical Library

Supplier: ChemBridge Corporation

LC STN Files: CHEMCATS

L9 ANSWER 2 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN

RN 695211-61-1 REGISTRY

ED Entered STN: 18 Jun 2004

CN Pyrimido[4,5-b]indolizine-3(4H)-acetic acid, 10-cyano-6,7,8,9-tetrahydro-4-oxo-(9CI) (CA INDEX NAME)

MF C13 H12 N4 O3

SR Chemical Library

Supplier: Chemical Block Ltd.

LC STN Files: CHEMCATS

ANSWER 1 OF 17 REGISTRY COPYRIGHT 2007 ACS on STN 907970-39-2 REGISTRY Entered STN: 20 Sep 2006 L9

RN

ED

CN INDEX NAME NOT YET ASSIGNED

MF C18 H16 N4 O S

SR Other Sources

Database: NCI 3D (National Cancer Institute)

10 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:633930 CAPLUS

DOCUMENT NUMBER: 141:157132

TITLE: Preparation of pyrrolopyrimidine derivatives useful as

modulators of multidrug resistance

INVENTOR(S): Milton, John; Wren, Stephen; Wang, Shouming; Folkes,

Adrian; Chuckowree, Irina; Hancox, Timothy; Miller,

Warren; Sohal, Sukhjit

PATENT ASSIGNEE(S): Xen

SOURCE:

Xenova Limited, UK

PCT Int. Appl., 114 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT N	KIN	D	DATE		APPLICATION NO.						DATE			
<del>-</del>														
WO 20040	A1	A1 20040805			WO 2004-GB274						20040123			
₩:	AE, AE,	AG, AL,	ΑL,	AM,	AM,	AM,	AT,	AT,	AU,	ΑU,	ΑZ,	ΑZ,	BA,	BB,
	BG, BG,	BR, BR,	BW,	BY,	BY,	ΒZ,	BZ,	CA,	CH,	CN,	CN,	co,	co,	CR,
	CR, CU,	CU, CZ,	CZ,	DE,	DE,	DK,	DK,	DM,	DZ,	EC,	EC,	EE,	EE,	EG,
	FI, FI,	GB,	GD,	GE,	GE,	GH,	GH,	GH,	GM,	HR,	HR,	HU,	HU,	
ID, IL, IN,			JΡ,	JP,	ΚE,	KE,	KG,	KG,	ΚP,	ΚP,	ΚP,	KR,	KR,	ΚZ,
	KZ, KZ,	LC, LK,	LR,	LS,	LS,	LT,	LU,	LV,	MA,	MD,	MD,	MG,	MK,	MN,
	MW, MX,	MX, MZ												
PRIORITY APPI	:	GB 2003-1736							A 20030124					
OTHER SOURCE	MAR	MARPAT 141:157132												
GI														

$$H_2C - CH_2 - F$$
 $NR^2R^6$ 
 $R^3$ 
 $N$ 
 $R^5$ 
 $R^5$ 
 $R^5$ 
 $R^5$ 
 $R^6$ 
 $R^7$ 
 $R^7$ 

Pyrrolopyrimidines of formula I [R1 = H, alkylaryl, alkyl, halo, etc.; R2, R6 = alkyl; NR2R6 = (substituted) 5 to 8-membered ring; R3, R4 = H, alkyl, alkylaryl; R3R4 = alkylene; R5 = CN, (substituted) CO2H, (substituted) CONH2, hydroxyalkyl, etc.] are prepared These compds. have activity as inhibitors of MRP (multidrug resistant protein) and may thus be used to modulate multidrug resistance, for instance in potentiating the cytotoxicity of a chemotherapeutic agent. Thus, II was prepared, and was an effective inhibitor of LTC4 transport by MRP1 at 0.7  $\mu$ M.

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrrolopyrimidine derivs. as modulators of multidrug resistance)

RN 132994-09-3 CAPLUS

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 731825-96-0 CAPLUS

CN Pyrimido[4,5-b]indolizin-4(1H)-one, 10-(4,5-dimethyl-2-thiazolyl)-6,7,8,9-tetrahydro-(9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

🛝 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:102825 CAPLUS

DOCUMENT NUMBER: 140:296874

TITLE: Studies on Pyrrolopyrimidines as Selective Inhibitors

of Multidrug-Resistance- Associated Protein in

Multidrug Resistance

AUTHOR(S): Wang, Shouming; Folkes, Adrian; Chuckowree, Irina;

Cockcroft, Xiaoling; Sohal, Sukhjit; Miller, Warren; Milton, John; Wren, Stephen P.; Vicker, Nigel;

Depledge, Paul; Scott, John; Smith, Lyndsay; Jones, Hazel; Mistry, Prakash; Faint, Richard; Thompson,

Deanne; Cocks, Simon

CORPORATE SOURCE: Department of Medicinal Chemistry, Department of

Pharmacology, Analytical Department, Xenova Ltd.,

Berkshire, SL1 4NL, UK

SOURCE: Journal of Medicinal Chemistry (2004) 47(6),

1329-1338

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:296874

Multidrug resistance mediated by P-glycoprotein (Pgp) or multidrug-resistance-associated protein (MRP) remains a major obstacle for successful treatment of cancer. Inhibition of Pgp and MRP transport is important for high efficacy of anticancer drugs. While several Pgp inhibitors have entered clin. trials, the development of specific MRP1 inhibitors is still in its infancy. In our screening program, we have identified a pyrrolopyrimidine (4) as a novel and selective MRP1 inhibitor. Subsequent SAR work on the 4-position of the template revealed the phenethylpiperazine side chain as a potent replacement of the benzylthio group of the lead mol. Introduction of groups at the 2-position seems to have no detrimental effect on activity. Modifications to the nitrile group at the 7-position resulted in the identification of analogs with groups, such as amides, with superior pharmacokinetic profiles. In vivo efficacy has been demonstrated by xenograft studies on selected compds.

IT 132994-09-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure-activity relationship studies of pyrrolopyrimidines as selective inhibitors of multidrug-resistance-associated protein in antitumor drug resistance)

RN 132994-09-3 CAPLUS

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

2003:678812 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 139:214483

Preparation of pyrrolopyrimidine derivatives as GSK-3 STITLE:

inhibitors

Kataoka, Kenichiro; Kosugi, Tomomi; Ishii, Toshihiro;  $\sqrt{I}$  INVENTOR(S):

Takeuchi, Takahiro; Tsutsumi, Takaharu; Nakano, Akira; Yamamoto, Yoji; Yoshioka, Noboru
Teijin Limited, Japan

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 210 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.					KIND DATE			APPLICATION NO.					DATE					
WO	WO 2003070730					A1 20030828						20030224						
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
-		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	
		PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,	
		UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	zw							
	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,	
		KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	
		FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,	
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG		
	CA 2477117								CA 2003-2477117									
	AU 2003211428																	
EP	EP 1477490			A1	A1 20041117				EP 2003-707009					20030224				
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		•	•		•		RO,			•	•		•					
	BR 2003007588																	
	CN 1646535																	
US	US 2005171094				A1	A1 20050804			US 2003-505228									
PRIORIT	PRIORITY APPLN. INFO.:									JP 2						0020		
										WO 2	003-	JP19	78	1	W 2	0030	224	
OTHER S	OTHER SOURCE(S):				MAR	PAT	Г 139:214483							•				
GI	GI																	

The title pyrrolopyrimidine derivs. with general formula of I [wherein X = AB O or S; n = 0-2; A = N or CH; GO = (un) substituted CH2, 2 valence group of (un) substituted benzene, furan, thiophene, pyrrole, isoxazole, cyclopentane, or cyclohexane; G1 = a single bond, CO2, CO, SO2, (un) substituted CONH, CSNH, or CONHSO2; R3 = a single bond, (un) substituted aliphatic (cyclo) hydrocarbyl, aromatic hydrocarbyl, or heterocyclyl; R4 = a single bond, aliphatic cyclohydrocarbyl, aromatic hydrocarbyl, or heterocyclyl; G2 = H, CO2H, CONHOH, SO3H, or tetrazol-5-yl] and pharmaceutically acceptable salts thereof are prepared as glycogen synthetase kinase 3 (GSK-3) inhibitors. For example, the compound II was prepared in a multi-step synthesis in good yield. Some of compds. I showed IC50 of <50 nM against GSK-3. I are useful as remedies or preventives for diseases in which GSK-3 participates such as diabetes, ·diabetic complications, Alzheimer's disease, neurodegenerative disease, depression, traumatic brain injury, hair loss, inflammatory diseases, cancer, immunodeficiency (no data). Formulations containing I as an active ingredient were also described.

IT 590386-69-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (drug candidate; preparation of pyrrolopyrimidine derivs. as GSK-3 inhibitors)

RN 590386-69-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

#### HCl

IT 473997-91-0P 473998-24-2P 473998-31-1P 590386-66-6P 590386-67-7P 590386-68-8P 590386-70-2P 590386-71-3P 590386-72-4P 590386-73-5P 590386-74-6P 590386-76-8P 590386-77-9P 590386-78-0P 590386-79-1P 590386-80-4P 590386-81-5P 590386-82-6P 590386-83-7P 590386-85-9P 590386-86-0P 590386-87-1P 590386-88-2P 590386-89-3P 590386-90-6P 590386-91-7P 590386-92-8P 590386-93-9P 590386-94-0P 590386-95-1P 590386-96-2P 590386-97-3P 590386-98-4P 590386-99-5P 590387-00-1P 590387-01-2P 590387-02-3P 590387-03-4P 590387-04-5P 590387-05-6P 590387-06-7P 590387-07-8P 590387-08-9P 590387-09-0P 590387-10-3P 590387-11-4P 590387-12-5P 590387-13-6P 590387-14-7P 590387-15-8P 590387-16-9P 590387-17-0P 590387-18-1P 590387-19-2P 590387-20-5P 590387-21-6P 590387-22-7P 590387-23-8P 590387-24-9P 590387-25-0P 590387-26-1P 590387-27-2P 590387-28-3P 590387-29-4P 590387-30-7P 590387-31-8P 590387-32-9P 590387-33-0P 590387-34-1P 590387-35-2P 590387-36-3P 590387-37-4P 590387-38-5P 590387-39-6P 590387-40-9P 590387-41-0P 590387-42-1P 590387-43-2P 590387-44-3P 590387-45-4P 590387-46-5P 590387-47-6P 590387-48-7P 590387-49-8P 590387-50-1P 590387-51-2P 590387-52-3P 590387-53-4P 590387-54-5P 590387-55-6P 590387-56-7P 590387-57-8P 590387-58-9P 590387-59-0P 590387-60-3P 590387-61-4P 590387-62-5P 590387-63-6P 590387-64-7P 590387-65-8P 590387-66-9P 590387-67-0P 590387-68-1P 590387-69-2P 590387-70-5P 590387-71-6P 590387-72-7P 590387-73-8P 590387-74-9P 590387-75-0P 590387-76-1P 590387-77-2P 590387-78-3P 590387-79-4P 590387-80-7P 590387-81-8P 590387-82-9P 590387-83-0P 590387-84-1P 590387-85-2P 590387-86-3P 590387-87-4P 590387-88-5P 590387-89-6P 590387-90-9P 590387-91-0P 590387-92-1P 590387-93-2P 590387-94-3P

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590387-95-4P 590387-96-5P 590387-97-6P
590387-98-7P 590387-99-8P 590388-00-4P
590388-01-5P 590388-02-6P 590388-03-7P
590388-04-8P 590388-05-9P 590388-06-0P
590388-07-1P 590388-08-2P 590388-09-3P
590388-10-6P 590388-11-7P 590388-12-8P
590388-13-9P 590388-14-0P 590388-15-1P
590388-16-2P 590388-17-3P 590388-18-4P
590388-19-5P 590388-20-8P 590388-21-9P
590388-22-0P 590388-23-1P 590388-24-2P
590388-25-3P 590388-26-4P 590388-27-5P
590388-28-6P 590388-29-7P 590388-30-0P
590388-31-1P 590388-32-2P 590388-33-3P
590388-34-4P 590388-35-5P 590388-36-6P
590388-37-7P 590388-38-8P 590388-39-9P
590388-40-2P 590388-41-3P 590388-42-4P
590388-43-5P 590388-44-6P 590388-45-7P
590388-46-8P 590388-47-9P 590388-48-0P
590388-49-1P 590388-50-4P 590388-51-5P
590388-52-6P 590388-53-7P 590388-54-8P
590388-55-9P 590388-56-0P 590388-57-1P
590388-58-2P 590388-59-3P 590388-60-6P
590388-61-7P 590388-62-8P 590388-63-9P
590388-64-0P 590388-65-1P 590388-66-2P
590388-67-3P 590388-68-4P 590388-69-5P
590388-70-8P 590388-71-9P 590388-72-0P
590388-73-1P 590388-74-2P 590388-75-3P
590388-76-4P 590388-77-5P 590388-78-6P
590388-79-7P 590388-80-0P 590388-81-1P
590388-82-2P 590388-83-3P 590388-84-4P
590388-85-5P 590388-86-6P 590388-87-7P
590388-88-8P 590388-89-9P 590388-90-2P
590388-91-3P 590388-92-4P 590388-93-5P
590388-94-6P 590388-95-7P 590388-96-8P
590388-97-9P 590388-98-0P 590388-99-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; preparation of pyrrolopyrimidine derivs. as GSK-3
   inhibitors)
473997-91-0 CAPLUS
1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-10-methyl-4-thioxo- (9CI) (CA INDEX NAME)
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RN

CN

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RN 473998-24-2 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)
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RN 473998-31-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(phenylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590386-66-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxylic acid, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 590386-67-7 CAPLUS

CN Pyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidine-8(1H)-carboxylic acid, 10-cyano-4,6,7,9-tetrahydro-4-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 590386-68-8 CAPLUS

CN 5H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]benzodiazepine-13-carbonitrile, 6,7,9,10-tetrahydro-9-oxo-5-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 590386-70-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-8-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

RN 590386-71-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(4-methylbenzoyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590386-72-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(4-methylphenyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & CN & H \\ \hline \\ NH-C-N & N & N \\ \hline \\ O & O \\ \end{array}$$

RN 590386-73-5 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-methoxyphenyl)sulfonyl]-4-oxo- (9CI) (CA INDEX NAME)

RN 590386-74-6 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-ll-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-8-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_{2} \xrightarrow{N} \xrightarrow{N} \stackrel{H}{\underset{N}{\bigvee}} N$$

RN 590386-76-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo-8-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

RN 590386-77-9 CAPLUS

CN 5H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]benzodiazepine-13-carbonitrile, 6,7,9,10-tetrahydro-5-(phenylmethyl)-9-thioxo-(9CI) (CA INDEX NAME)

RN 590386-78-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-benzoyl-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ H & N \\ \hline \\ O & S \end{array}$$

RN 590386-79-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-(cyanoacetyl)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590386-80-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(4-methylphenyl)-4-thioxo-(9CI) (CAINDEX NAME)

RN 590386-81-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(phenylsulfonyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590386-82-6 CAPLUS

CN Benzoic acid, 3-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 590386-83-7 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[3-[(hydroxyamino)carbonyl]phenyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590386-85-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-10-methyl-8-(phenylmethyl)-4-thioxo-(9CI) (CA INDEX NAME)

$$Ph-CH2 \xrightarrow{Me} CN \xrightarrow{H} N$$

RN 590386-86-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-acetyl-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590386-87-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-8-(phenylacetyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C$$

$$O$$

$$O$$

$$O$$

$$O$$

$$O$$

$$O$$

$$O$$

RN 590386-88-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-8-(1-oxo-2-phenylbutyl)- (9CI) (CA INDEX NAME)

RN 590386-89-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(3-methoxyphenyl)acetyl]-4-oxo- (9CI) (CA INDEX NAME)

RN 590386-90-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-methoxyphenyl)acetyl]-4-oxo- (9CI) (CA INDEX NAME)

MeO 
$$CH_2-C-N$$
  $N$   $N$   $N$   $N$ 

RN 590386-91-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(3,4-dimethoxyphenyl)acetyl]-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

MeO 
$$CH_2-C-N$$
  $N$   $N$ 

RN 590386-92-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(4-chlorophenyl)acetyl]-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

$$C1 \longrightarrow CH_2 - C \longrightarrow N \longrightarrow N \longrightarrow N$$

RN 590386-93-9 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-8-[[4-(phenylmethoxy)phenyl]acetyl]- (9CI) (CA INDEX NAME)

RN 590386-94-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-benzoyl-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ N & N \\ N & N \\ O & O \end{array}$$

RN 590386÷95-1 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(1-naphthalenylcarbonyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590386-96-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-naphthalenylcarbonyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline \\ C - N & N \\ \hline \\ O \end{array}$$

RN 590386-97-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(3-methylbenzoyl)-4-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ N & N \\ \hline \end{array}$$

RN 590386-98-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-methoxybenzoyl)-4-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline C & N & N \\ \hline OMe & O \\ \end{array}$$

RN 590386-99-5 CAPLUS

## 10/505,228

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(3-methoxybenzoyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ N & N \\ \hline \end{array}$$

RN 590387-00-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(4-methoxybenzoyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-01-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[3-(dimethylamino)benzoyl]-4,6,7,8,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ N & N \\ \hline \\ C & N & N \\ \hline \\ O & \\ \end{array}$$

RN 590387-02-3 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-nitrobenzoyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
CN & H \\
N & N \\
NO_2 & O
\end{array}$$

RN 590387-03-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(3-nitrobenzoyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline \\ C - N & N \\ \hline \end{array}$$

RN 590387-04-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(4-nitrobenzoyl)-4-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline \\ C - N & N \end{array}$$

RN 590387-05-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-(3-cyanobenzoyl)-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-06-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,

8-(4-cyanobenzoyl)-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-07-8 CAPLUS

CN Benzoic acid, 4-[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & CN & H \\ \hline \\ MeO-C & O & N & N \\ \hline \\ \\ C-N & N \\ \\ O & \\ \end{array}$$

RN 590387-08-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-8-(2-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

RN 590387-09-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-8-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

RN 590387-10-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-8-(4-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline \\ C & N & N \\ \hline \end{array}$$

RN 590387-11-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-chloro-3-pyridinyl)carbonyl]-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
CN & H \\
N & C & N & N \\
\end{array}$$

RN 590387-12-5 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(6-chloro-3-pyridinyl)carbonyl]-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & CN & H \\ N & C - N & N \end{array}$$

RN 590387-13-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(1-methylethyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-14-7 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$Ph-CH_2-NH-C$$

$$O$$

$$O$$

$$O$$

$$O$$

RN 590387-15-8 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[(2-methylphenyl)methyl]-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-16-9 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[(3-methylphenyl)methyl]-4-oxo- (9CI) (CA INDEX NAME)

Me 
$$CH_2-NH-C-N$$
  $N$   $N$   $N$   $N$ 

RN 590387-17-0 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[(4-methylphenyl)methyl]-4-oxo- (9CI) (CA INDEX NAME)

Me 
$$CH_2-NH-C-N$$
  $N$   $N$   $N$   $N$ 

RN 590387-18-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[(4-methoxyphenyl)methyl]-4-oxo- (9CI) (CA INDEX NAME)

MeO 
$$CH_2-NH-C-N$$
  $N$   $N$   $N$   $N$ 

RN 590387-19-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[(2-fluorophenyl)methyl]-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-20-5 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[(3-fluorophenyl)methyl]-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-21-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[(4-fluorophenyl)methyl]-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-22-7 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-[(2-chlorophenyl)methyl]-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-23-8 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[(2,4-dichlorophenyl)methyl]-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

$$C1 \qquad CH_2-NH-C-N \qquad N \qquad N \qquad N$$

RN 590387-24-9 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[(3,4-dichlorophenyl)methyl]-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & CN & H \\ \hline \\ C1 & CH_2-NH-C-N & N & N \\ \hline \\ \\ O & \\ \end{array}$$

RN 590387-25-0 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-phenyl- (9CI) (CA INDEX NAME)

RN 590387-26-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-[1,1'-biphenyl]-4-yl-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-27-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-1-naphthalenyl-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-28-3 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-2-naphthalenyl-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-29-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(2-methylphenyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 590387-30-7 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(3-methylphenyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ NH-C-N & N \end{array}$$

RN 590387-31-8 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(2-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-32-9 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(3-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ NH-C-N & N \end{array}$$

RN 590387-33-0 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(4-methoxyphenyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-34-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,5-dimethoxyphenyl)-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 590387-35-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,4-dimethoxyphenyl)-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-36-3 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-1,3-benzodioxol-5-yl-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline \\ NH-C-N & N \\ \hline \\ \end{array}$$

RN 590387-37-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-[4-(trifluoromethoxy)phenyl]-(9CI) (CA INDEX NAME)

RN 590387-38-5 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 590387-39-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-(2-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 590387-40-9 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-(3-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 590387-41-0 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 590387-42-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[4-(dimethylamino)phenyl]-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ \text{Me}_2 \text{N} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$$

RN 590387-43-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(2-nitrophenyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-44-3 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(3-nitrophenyl)-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ NH-C-N & N \end{array}$$

RN . 590387-45-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(4-nitrophenyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-46-5 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-(4-chloro-3-nitrophenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 590387-47-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,5-dinitrophenyl)-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 590387-48-7 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3-cyanophenyl)-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-49-8 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(4-cyanophenyl)-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-50-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-(4-acetylphenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-51-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 590387-52-3 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 590387-53-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(2-fluorophenyl)-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-54-5 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3-fluorophenyl)-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-55-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(4-fluorophenyl)-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-56-7 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,5-difluorophenyl)-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 590387-57-8 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-(2-chlorophenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & CN & H \\ NH-C-N & N-N \\ \end{array}$$

RN 590387-58-9 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-(3-chlorophenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-59-0 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-(4-chlorophenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & CN & H \\ \hline \\ NH-C-N & N & N \\ \hline \\ O & \\ \end{array}$$

RN 590387-60-3 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,4-dichlorophenyl)-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & CN & H\\ \hline \\ NH-C-N & N & N \\ \hline \\ \end{array}$$

RN 590387-61-4 CAPLUS

CN Benzoic acid, 2-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 590387-62-5 CAPLUS

CN Benzoic acid, 3-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline \\ MeO-C & NH-C-N & N \\ \hline \\ \\ \end{array}$$

RN 590387-63-6 CAPLUS

CN Benzoic acid, 4-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & & & & CN & H \\
MeO-C & & & & & & \\
NH-C-N & & & & & \\
\end{array}$$

RN 590387-64-7 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, dimethyl ester (9CI) (CA INDEX NAME)

RN 590387-65-8 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(2,4-difluorophenyl)-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 590387-66-9 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,4-difluorophenyl)-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 590387-67-0 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,5-dichlorophenyl)-1,4,6,7,9,10-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 590387-68-1 CAPLUS

CN Benzoic acid, 2-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 590387-69-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-methylphenyl)sulfonyl]-4-oxo- (9CI) (CA INDEX NAME)

RN 590387-70-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-nitrophenyl)sulfonyl]-4-oxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} c & c & H \\ c & N & N \\ c & N \\ c & N \end{array}$$

RN 590387-71-6 CAPLUS

CN Benzamide, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 590387-72-7 CAPLUS

CN Benzamide, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)sulfonyl]-4-methyl-(9CI) (CA INDEX NAME)

RN 590387-73-8 CAPLUS

CN Benzamide, 2-chloro-N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & CN & H \\ C-NH-S-N & N-N-N \\ C1 & O & O \\ \end{array}$$

RN 590387-74-9 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-ll-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(phenylacetyl)-4-thioxo- (9CI) (CA INDEX NAME)

$$Ph-CH_2-C-N N N N N$$

RN 590387-75-0 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-ll-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(1-oxo-3-phenylpropyl)-4-thioxo- (9CI) (CA\_INDEX\_NAME)

RN 590387-76-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(phenylmethyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 590387-77-2 CAPLUS

CN L-Glutamic acid, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 590387-78-3 CAPLUS

CN β-Alanine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 590387-79-4 CAPLUS

CN L-Methionine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 590387-80-7 CAPLUS

CN L-Serine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]-O-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 590387-81-8 CAPLUS

CN Hexanoic acid, 6-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 590387-82-9 CAPLUS

CN Glycine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 590387-83-0 CAPLUS

CN Butanoic acid, 4-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 590387-84-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[(4-methoxyphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590387-85-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[(2-fluorophenyl)methyl]-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590387-86-3 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[(3-fluorophenyl)methyl]-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590387-87-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-[(2-chlorophenyl)methyl]-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590387-88-5 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-[(2,4-dichlorophenyl)methyl]-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & CN & H \\ CH_2-NH-C-N & N-N-N \\ \end{array}$$

RN 590387-89-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-phenyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 590387-90-9 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-2-naphthalenyl-4-thioxo- (9CI) (CAINDEX NAME)

RN 590387-91-0 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(2-methylphenyl)-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & CN & H \\ \hline & NH-C-N & N-N \\ \hline & S \end{array}$$

RN 590387-92-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(3-methylphenyl)-4-thioxo-(9CI) (CPINDEX NAME)

$$\begin{array}{c|c} CN & H \\ NH-C-N & N \\ \end{array}$$

RN 590387-93-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(3-methoxyphenyl)-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ NH-C-N & N \\ \end{array}$$

RN 590387-94-3 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(4-methoxyphenyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 590387-95-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,4-dimethoxyphenyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590387-96-5 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-N-[4-(trifluoromethoxy)phenyl]-(9CI) (CA INDEX NAME)

RN 590387-97-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(3-nitrophenyl)-4-thioxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ NH-C-N & N \end{array}$$

RN 590387-98-7 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-(2-chlorophenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590387-99-8 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-(4-chlorophenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-00-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(phenylmethyl)-4-thioxo-(9CI) (CA INDEX NAME)

$$Ph-CH_2-NH-C$$

$$S$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

RN 590388-01-5 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(2-phenylethyl)-4-thioxo-(9CI) (CA INDEX NAME)

$$Ph-CH_2-CH_2-NH-C$$

$$S$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

RN 590388-02-6 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-phenyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-03-7 CAPLUS

CN Benzoic acid, 4-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & CN & H\\ MeO-C & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 590388-04-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-phenylethyl)-4-thioxo-(9CI) (CA INDEX NAME)

$$Ph-CH_2-CH_2 \xrightarrow{N} \xrightarrow{N} \xrightarrow{N} S$$

RN 590388-05-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-methylphenyl)methyl]-4-thioxo- (9CI) (CA INDEX NAME)

$$Me$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590388-06-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(2-methoxyphenyl)methyl]-4-thioxo- (9CI) (CA INDEX NAME)

## 10/505,228

RN 590388-07-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(3-methoxyphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

MeO 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590388-08-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-methoxyphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline \\ CH_2 - N & N \\ \hline \\ S \end{array}$$

RN 590388-09-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-fluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$CH_2$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590388-10-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(3-fluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \hline \\ CH_2 - N & N \\ \hline \\ S \end{array}$$

RN 590388-11-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(4-fluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-12-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-hydroxyphenyl)methyl]-4-thioxo- (9CI) (CA INDEX NAME)

HO 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590388-13-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-chlorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-14-0 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-ll-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-naphthalenylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-15-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(1-naphthalenylmethyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-16-2 CAPLUS

CN Pyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidine-10-carbonitrile, 8-acetyl-1,4,6,7,8,9-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 590388-17-3 CAPLUS

CN Pyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidine-10-carbonitrile,
1,4,6,7,8,9-hexahydro-4-oxo-8-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

RN 590388-18-4 CAPLUS

CN Pyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidine-10-carbonitrile, 8-benzoyl-1,4,6,7,8,9-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590388-19-5 CAPLUS

CN Pyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidine-8(1H)-carboxamide, 10-cyano-4,6,7,9-tetrahydro-N-(1-methylethyl)-4-oxo- (9CI) (CA INDEX NAME)

RN 590388-20-8 CAPLUS

CN Pyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidine-8(1H)-carboxamide, 10-cyano-4,6,7,9-tetrahydro-4-oxo-N-phenyl- (9CI) (CA INDEX NAME)

RN 590388-21-9 CAPLUS

CN Pyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-thioxo-8-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

RN 590388-22-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(methoxyacetyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-23-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[3-(1H-imidazol-4-yl)-1-oxo-2-propenyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$CH = CH - C - N N - N N$$

RN 590388-24-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-butanamide, 11-cyano-1,4,6,7,9,10-hexahydro-N,N-dimethyl- $\gamma$ -oxo-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-25-3 CAPLUS

CN Acetamide, N-[2-(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)-2-oxoethyl]- (9CI) (CA INDEX NAME)

RN 590388-26-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[(aminocarbonyl)amino]acetyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-27-5 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[2-(formylamino)-1-oxopropyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-28-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[2-[(aminocarbonyl)amino]-1-oxopropyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-29-7 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-butanamide,
11-cyano-1,4,6,7,9,10-hexahydro-γ-oxo-4-thioxo- (9CI) (CA INDEX
NAME)

RN 590388-30-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[3-[(aminocarbonyl)amino]-1-oxopropyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-31-1 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-pentanoic acid, 11-cyano- $\gamma$ -[[(1,1-dimethylethoxy)carbonyl]amino]-1,4,6,7,9,10-hexahydro- $\delta$ -oxo-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-32-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-pentanoic acid, 11-cyano- $\gamma$ -[[(1,1-dimethylethoxy)carbonyl]amino]-1,4,6,7,9,10-hexahydro- $\delta$ -oxo-4-thioxo-, ( $\gamma$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 590388-33-3 CAPLUS

Absolute stereochemistry.

RN 590388-34-4 CAPLUS

Absolute stereochemistry.

RN 590388-35-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(1H-indol-3-yloxoacetyl)-4-oxo- (9CI) (CA INDEX NAME)

$$O = C - C - N N N N$$

RN 590388-36-6 CAPLUS

CN β-Alanine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 590388-37-7 CAPLUS

CN Methionine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]- (9CI) (CA INDEX NAME)

590388-38-8 CAPLUS RN

Hexanoic acid, 6-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-CN pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]- (9CI) (CA INDEX NAME)

590388-39-9 CAPLUS RN

Glycine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-CN pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]- (9CI) (CA INDEX NAME)

590388-40-2 CAPLUS RN

Butanoic acid, 4-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-CN pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 590388-41-3 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-1,4,6,7,9,10-hexahydro-N-[(2-methylphenyl)methyl]-4-thioxo- (9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} & CN & H \\ \hline \\ CH_2-NH-C-N & N-N \\ \hline \\ S & S \\ \end{array}$$

RN 590388-42-4 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-1,4,6,7,9,10-hexahydro-N-[(3-methylphenyl)methyl]-4-thioxo-(9CI)
(CA INDEX NAME)

Me 
$$CH_2-NH-C-N$$
  $N$   $N$   $N$   $N$   $N$ 

RN 590388-43-5 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-1,4,6,7,9,10-hexahydro-N-[(4-methylphenyl)methyl]-4-thioxo- (9CI)
(CA INDEX NAME)

RN 590388-44-6 CAPLUS CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3,5-dimethoxyphenyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-45-7 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-1,4,6,7,9,10-hexahydro-N-(3-phenoxyphenyl)-4-thioxo-(9CI) (CA
INDEX NAME)

RN 590388-46-8 CAPLUS CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(4-phenoxyphenyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-47-9 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-N-[4-(dimethylamino)phenyl]-1,4,6,7,9,10-hexahydro-4-thioxo(9CI) (CA INDEX NAME)

590388-48-0 CAPLUS RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(2-nitrophenyl)-4-thioxo-(9CI) CN (CA INDEX NAME)

590388-49-1 CAPLUS RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, N-(4-chloro-3-nitrophenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) CN (CA INDEX NAME)

590388-50-4 CAPLUS

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, RN 11-cyano-N-(3,5-dinitrophenyl)-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) CN (CA INDEX NAME)

590388-51-5 CAPLUS

RN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, CN 11-cyano-N-(4-cyanophenyl)-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-52-6 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
N-(4-acetylphenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA
INDEX NAME)

RN 590388-53-7 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-N-[2-(trifluoromethyl)phenyl](9CI) (CA INDEX NAME)

RN 590388-54-8 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-N-(2-fluorophenyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA
INDEX NAME)

RN 590388-55-9 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(3-fluorophenyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-56-0 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(4-fluorophenyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-57-1 CAPLUS

CN Benzoic acid, 3-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 590388-58-2 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]-, dimethyl ester (9CI) (CA INDEX NAME)

RN 590388-59-3 CAPLUS CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, 11-cyano-N-(2,4-difluorophenyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
F & O & H \\
NH-C-N & N
\end{array}$$

RN 590388-60-6 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-N-(3,4-difluorophenyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI)
(CA INDEX NAME)

RN 590388-61-7 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide,
11-cyano-N-(3,5-dichlorophenyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} C1 & CN & H \\ \hline \\ NH-C-N & N \\ \hline \\ S \end{array}$$

RN 590388-62-8 CAPLUS
CN Benzoic acid, 3-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8Hpyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]- (9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

Absolute stereochemistry.

RN 590388-64-0 CAPLUS
CN D-Serine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]-O-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 590388-65-1 CAPLUS
CN Benzoic acid, 4-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]- (9CI)
(CA INDEX NAME)

HO<sub>2</sub>C 
$$O$$
  $N$   $N$   $N$   $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590388-66-2 CAPLUS
CN Benzoic acid, 2-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]amino]- (9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} CO_2H & CN & H \\ \hline NH-C-N & N-N & N \\ \hline \end{array}$$

RN 590388-67-3 CAPLUS CN L-Alanine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8Hpyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

590388-68-4 CAPLUS RN

L-Leucine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-CN pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

590388-69-5 CAPLUS RN

L-Phenylalanine, N-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-CN pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

590388-70-8 CAPLUS RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carboxamide, CN N-benzoyl-11-cyano-1,4,6,7,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

590388-71-9 CAPLUS RN

Benzoic acid, 2-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-CN pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & CN & H \\ C-OMe & NH-C-N & N & N \\ S & S & S \end{array}$$

590388-72-0 CAPLUS RN

Benzoic acid, 3-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-CN pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ \parallel & \parallel & \parallel \\ NH-C-N & N & N \\ \end{array}$$

590388-73-1 CAPLUS RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, CN 11-cyano-1,4,6,7,9,10-hexahydro-N-3-pyridinyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 590388-74-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-(3-pyridinylmethyl)-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & CN \\ & & & \\ N & & & \\ & & & \\ N & & & \\ & & & \\ N & & & \\ & & & \\ N & & & \\ & & & \\ N & & & \\ & & & \\ N & & \\$$

RN 590388-75-3 CAPLUS

CN Benzenesulfonic acid, 4-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]-(9CI) (CA INDEX NAME)

RN 590388-76-4 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[(tetrahydro-2-furanyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-77-5 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-N-(2-furanylmethyl)-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
CN & H \\
N & N
\end{array}$$

590388-78-6 CAPLUS 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, RN N-[4-(aminosulfonyl)phenyl]-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-CN (CA INDEX NAME)

590388-79-7 CAPLUS Carbamic acid, [4-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-RN

pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-CN

yl)thioxomethyl]amino]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

590388-80-0 CAPLUS Benzoic acid, 3-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-oxo-8H-RNpyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]-CN(9CI) (CA INDEX NAME)

HO2C 
$$NH-C-N$$
  $N$   $N$   $N$ 

RN 590388-81-1 CAPLUS
CN Benzoic acid, 3-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino](9CI) (CA INDEX NAME)

HO<sub>2</sub>C 
$$NH-C-N$$
  $N$   $N$   $N$   $N$ 

RN 590388-82-2 CAPLUS

Benzoic acid, 4-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]-(9CI) (CA INDEX NAME)

RN 590388-83-3 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide,
11-cyano-1,4,6,7,9,10-hexahydro-N-[2-(1-piperidinyl)ethyl]-4-thioxo- (9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ N \longrightarrow CH_2 - CH_2 - NH - C \longrightarrow N & & N \longrightarrow N \\ & & & \\ & & & \\ S & & & \\ \end{array}$$

RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-N-[4-(dimethylamino)-1-naphthalenyl]-1,4,6,7,9,10-hexahydro-4-CN thioxo- (9CI) (CA INDEX NAME)

Benzoic acid, 2-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-RNpyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]-CN (9CI) (CA INDEX NAME)

590388-86-6 CAPLUS

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, RN 11-cyano-1,4,6,7,9,10-hexahydro-N-(2-methoxyethyl)-4-thioxo- (9CI) (CA CN INDEX NAME)

590388-87-7 CAPLUS

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, RN 11-cyano-1,4,6,7,9,10-hexahydro-N-(3-methoxypropyl)-4-thioxo-(9CI) CN INDEX NAME)

RN 590388-88-8 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[3-(4-morpholinyl)propyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590388-89-9 CAPLUS

CN Butanoic acid, 3-[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]-(9CI) (CA INDEX NAME)

RN 590388-90-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, N-(2-aminoethyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

590388-91-3 CAPLUS RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, CN N-(3-aminopropyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

590388-92-4 CAPLUS RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, CN N-(4-aminobutyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

590388-93-5 CAPLUS RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, CN N-(5-aminopentyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

. 
$$H_2N-(CH_2)_5-NH-C$$
S
$$N$$
S
$$N$$
S

590388-94-6 CAPLUS RN

8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, CN N-(4-aminophenyl)-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI) (CA) INDEX NAME)

RN 590388-95-7 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide,
N-[4-(aminomethyl)phenyl]-11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo- (9CI)
(CA INDEX NAME)

$$H_2N-CH_2$$
 $S$ 
 $NH-C-N$ 
 $N$ 
 $S$ 
 $S$ 

RN 590388-96-8 CAPLUS
CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide,
11-cyano-N-[3-(diethylamino)propyl]-1,4,6,7,9,10-hexahydro-4-thioxo-(9CI)
(CA INDEX NAME)

$$Et_{2}N-(CH_{2})_{3}-NH-C$$

$$S$$

$$N$$

$$N$$

$$N$$

$$N$$

$$S$$

RN 590388-97-9 CAPLUS CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-butyl-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ N & N \\ \end{array}$$

RN 590388-98-0 CAPLUS

1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,

8-[(3,4-dimethoxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI)

(CA INDEX NAME)

MeO 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590388-99-1 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[[4-(phenylmethoxy)phenyl]methyl]-4-thioxo- (9CI)
(CA INDEX NAME)

$$Ph-CH_2-O$$

$$CH_2-N$$

$$S$$

590389-00-7P 590389-01-8P 590389-02-9P IT 590389-03-0P 590389-04-1P 590389-05-2P 590389-06-3P 590389-07-4P 590389-08-5P 590389-09-6P 590389-10-9P 590389-11-0P 590389-13-2P 590389-15-4P 590389-16-5P 590389-17-6P 590389-18-7P 590389-19-8P 590389-20-1P 590389-21-2P 590389-22-3P 590389-23-4P 590389-24-5P 590389-25-6P 590389-26-7P 590389-27-8P 590389-28-9P 590389-29-0P 590389-30-3P 590389-31-4P 590389-32-5P 590389-33-6P 590389-34-7P 590389-35-8P 590389-36-9P 590389-37-0P 590389-38-1P 590389-39-2P 590389-40-5P 590389-41-6P 590389-42-7P 590389-43-8P 590389-44-9P 590389-45-0P 590389-46-1P 590389-47-2P 590389-48-3P 590389-49-4P 590389-50-7P 590389-51-8P 590389-52-9P 590389-53-0P 590389-54-1P 590389-55-2P 590389-56-3P 590389-57-4P 590389-58-5P 590389-59-6P 590389-60-9P 590389-61-0P 590389-62-1P 590389-63-2P 590389-64-3P 590389-65-4P 590389-67-6P 590389-68-7P 590389-69-8P 590389-70-1P 590389-71-2P 590389-72-3P 590389-73-4P 590389-74-5P 590389-75-6P 590389-76-7P 590389-77-8P 590389-78-9P 590389-79-0P 590389-80-3P

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590389-81-4P 590389-82-5P 590389-83-6P
   590389-84-7P 590389-85-8P 590389-86-9P
   590389-87-0P 590389-88-1P 590389-89-2P
   590389-90-5P 590389-92-7P 590389-93-8P
   590389-95-0P 590389-97-2P 590389-98-3P
    590389-99-4P 590390-00-4P 590390-01-5P
    590390-02-6P 590390-03-7P 590390-04-8P
    590390-05-9P 590390-06-0P 590390-07-1P
    590390-08-2P 590390-09-3P 590390-10-6P
    590390-11-7P 590390-12-8P 590390-13-9P
    590390-14-0P 590390-15-1P 590390-16-2P
    590390-17-3P 590390-18-4P 590390-19-5P
    590390-20-8P 590390-21-9P 590390-22-0P
    590390-23-1P 590390-24-2P 590390-25-3P
    590390-26-4P 590390-27-5P 590390-28-6P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
    (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (drug candidate; preparation of pyrrolopyrimidine derivs. as GSK-3
     (Uses)
        inhibitors)
     1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
RN
     4,6,7,8,9,10-hexahydro-8-(3-pyridinylmethyl)-4-thioxo- (9CI) (CA INDEX
CN
     NAME)
```

RN 590389-01-8 CAPLUS CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(3-phenylpropyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-02-9 CAPLUS

CN Benzoic acid, 4-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8Hpyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)methyl]- (9CI) (CA
INDEX NAME)

RN 590389-03-0 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-(4-pyridinylmethyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-04-1 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[[3-(phenylmethoxy)phenyl]methyl]-4-thioxo-(9CI)
(CA INDEX NAME)

$$Ph-CH_2-O$$
 $CH_2-N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-05-2 CAPLUS

1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,

1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,

4,6,7,8,9,10-hexahydro-8-[[2-(phenylmethoxy)phenyl]methyl]-4-thioxo-(9CI)

(CA INDEX NAME)

RN 590389-06-3 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
8-[(2-cyanophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA
INDEX NAME)

RN 590389-07-4 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
8-[(3-cyanophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-08-5 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
8-(cyclohexylmethyl)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-09-6 CAPLUS

1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,

4,6,7,8,9,10-hexahydro-4-thioxo-8-[(3,4,5-trimethoxyphenyl)methyl]- (9CI)

(CA INDEX NAME)

RN 590389-10-9 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
8-(1,3-benzodioxol-5-ylmethyl)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$CH_2$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-11-0 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-(2-methylpropyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-13-2 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[(2-hydroxyphenyl)methyl]-4-thioxo- (9CI) (CA
INDEX NAME)

## 10/505,228

RN 590389-15-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(2-nitrophenyl)methyl]-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-16-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[[2-(2-hydroxyethoxy)phenyl]methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-17-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(3-nitrophenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$CH_2$$
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-18-7 CAPLUS

CN Benzoic acid, 2-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)methyl]- (9CI) (CA INDEX NAME)

$$CO_2H$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-19-8 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
8-[(5-chloro-2-nitrophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI)
(CA INDEX NAME)

NO2
$$CH_2 - N N N S$$

RN 590389-20-1 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
8-[(5-chloro-2-hydroxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo(9CI) (CA INDEX NAME)

RN 590389-21-2 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[(2-hydroxy-5-methoxyphenyl)methyl]-4-thioxo(9CI) (CA INDEX NAME)

RN 590389-22-3 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[(5-hydroxy-2-nitrophenyl)methyl]-4-thioxo- (9CI)
(CA INDEX NAME)

RN 590389-23-4 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-4-thioxo(9CI) (CA INDEX NAME)

$$CH_2$$
 $NO_2$ 
 $CN$ 
 $H$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-24-5 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
8-[[2-fluoro-6-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4thioxo- (9CI) (CA INDEX NAME)

RN 590389-25-6 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[(4-hydroxy-2-methoxyphenyl)methyl]-4-thioxo(9CI) (CA INDEX NAME)

OMe 
$$CH_2$$
  $N$   $N$   $N$   $N$ 

RN 590389-26-7 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[(5-nitro-2-furanyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$O_2N$$
 $O_2N$ 
 $O_2N$ 
 $O_3$ 
 $O_4$ 
 $O_4$ 
 $O_5$ 
 $O_5$ 
 $O_5$ 
 $O_5$ 
 $O_7$ 
 $O$ 

RN 590389-27-8 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-8-[(5-methyl-2-furanyl)methyl]-4-thioxo-(9CI) (CAINDEX NAME)

Me 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$ 

RN 590389-28-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[[5-(hydroxymethyl)-2-furanyl]methyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$HO-CH_2$$
 $O$ 
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-29-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-chloro-6-fluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$C1$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-30-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2,4-dimethoxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-31-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2,5-dimethoxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

590389-32-5 CAPLUS RN

1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, CN 8-[(3-fluoro-2-hydroxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

590389-33-6 CAPLUS RN

1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, CN 4,6,7,8,9,10-hexahydro-8-[(2-hydroxy-3-methoxyphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

MeO 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590389-34-7 CAPLUS

1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, CN 8-[(2,3-dihydroxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-35-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(2-hydroxy-4-methoxyphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

OH 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590389-36-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2,4-dihydroxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

OH 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590389-37-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo-8-[[2-(trifluoromethyl)phenyl]methyl]-(9CI) (CA INDEX NAME)

RN 590389-38-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(3-fluoro-4-methoxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

MeO 
$$CH_2$$
  $N$   $N$   $N$   $N$ 

RN 590389-39-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(3,5-dimethoxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & \text{CN} & \text{H} \\ \text{N} & \text{N} & \text{N} \\ \text{MeO} & \text{S} \end{array}$$

RN 590389-40-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(3-hydroxyphenyl)methyl]-4-thioxo- (9CI) (CA INDEX NAME)

HO 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590389-41-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(3-hydroxy-4-methoxyphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-42-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(3,4-dihydroxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

HO 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$ 

RN 590389-43-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo-8-[[3-(trifluoromethyl)phenyl]methyl]-(9CI) (CA INDEX NAME)

$$_{\text{F3C}}$$
  $_{\text{CH}_2}$   $_{\text{N}}$   $_{\text{N}}$   $_{\text{N}}$ 

RN 590389-44-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(4-cyanophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-45-0 CAPLUS

CN Acetamide, N-[4-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 590389-46-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-thienylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-47-2 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(3-methyl-2-thienyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-48-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(4-bromo-2-thienyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$S$$
 $CH_2$ 
 $N$ 
 $N$ 
 $S$ 
 $S$ 
 $S$ 
 $S$ 
 $S$ 
 $S$ 
 $S$ 

RN 590389-49-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(5-nitro-2-thienyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$O_2N$$
 $S$ 
 $CH_2$ 
 $N$ 
 $N$ 
 $S$ 
 $S$ 

RN 590389-50-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(5-methyl-2-thienyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-51-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(3-thienylmethyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-52-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-hydroxy-3-methoxyphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

HO 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$ 

RN 590389-53-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo-8-[[4-(trifluoromethyl)phenyl]methyl]-(9CI) (CA INDEX NAME)

$$_{\text{F}_3\text{C}}$$
  $_{\text{CH}_2}$   $_{\text{N}}$   $_{\text{N}}$   $_{\text{N}}$ 

RN 590389-54-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-methylbutyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-55-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(3-methylbutyl)-4-thioxo-(9CI) (CA INDEX NAME)

$$Me_2CH-CH_2-CH_2 \xrightarrow{N} \xrightarrow{N} \xrightarrow{N}$$

RN 590389-56-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(4,5-dimethoxy-2-nitrophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-57-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(3-methoxy-2-nitrophenyl)methyl]-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-58-5 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[3-(2-nitrophenyl)-2-propenyl]-4-thioxo- (9CI) (CA INDEX NAME)

$$NO_2$$
 $CH = CH - CH_2 - N$ 
 $N$ 
 $N$ 

RN 590389-59-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-chloro-5-nitrophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$CH_2$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-60-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(2-hydroxy-5-nitrophenyl)methyl]-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-61-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[3-(4-nitrophenyl)-2-propenyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$CH = CH - CH_2 - N$$
 $CH = CH - CH_2 - N$ 
 $CH = C$ 

RN 590389-62-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2,3-difluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CFINDEX NAME)

RN 590389-63-2 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2,4-difluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$F$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-64-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2,5-difluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$CH_2$$
 $N$ 
 $N$ 
 $S$ 

RN 590389-65-4 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(3,4-difluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CAINDEX NAME)

RN 590389-67-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-(3-furanylmethyl)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$O \longrightarrow CH_2 \longrightarrow N \longrightarrow N$$

RN 590389-68-7 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-ll-carbonitrile, 8-[(3-chloro-4-fluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-69-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(4-hydroxy-3-methylphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

HO 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$ 

RN 590389-70-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[[2-(2-propenyloxy)phenyl]methyl]-4-thioxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O-CH_2-CH = CH_2 & CN \\ \hline \\ CH_2-N & N \\ \hline \\ S \end{array}$$

RN 590389-71-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-(2-benzofuranylmethyl)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$CH_2$$

RN 590389-72-3 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[3-(4-methoxyphenyl)-2-propenyl]-4-thioxo-(9CI) (CA INDEX NAME)

MeO 
$$CH = CH - CH_2 - N N$$

RN 590389-73-4 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$CH_2 - N N N N$$

RN 590389-74-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(2-hydroxy-3-methylphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

Me 
$$CH_2$$
  $N$   $N$   $N$   $N$   $N$ 

RN 590389-75-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-fluoro-5-nitrophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-76-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-chloro-4-fluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$C1$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-77-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[[5-(3-nitrophenyl)-2-furanyl]methyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$O_2N$$
 $O_2N$ 
 $O_2N$ 
 $O_2N$ 
 $O_3N$ 
 $O_4N$ 
 $O_4N$ 
 $O_5N$ 
 $O_5N$ 

RN 590389-78-9 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-chloro-4-hydroxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-79-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[2-fluoro-3-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$F_{3}C$$
 $CH_{2}$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-80-3 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-ll-carbonitrile, 8-[[2-fluoro-4-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$F_{3}$$
CH<sub>2</sub>—N N N S

RN 590389-81-4 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[2-fluoro-5-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-82-5 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[4-fluoro-2-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$CF_3$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590389-83-6 CAPLUS

'CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[4-fluoro-3-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-84-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[3-(2-furanyl)-2-methyl-2-propenyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{O} \\
\text{CH} = \text{C-CH}_2 - \text{N} \\
\text{S}
\end{array}$$

RN 590389-85-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2-fluoro-5-methoxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-86-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(5-chloro-3-methyl-1-phenyl-1H-pyrazol-4-yl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-87-0 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[[5-(4-nitrophenyl)-2-furanyl]methyl]-4-thioxo-(9CI) (CA INDEX NAME)

$$O_2N$$
 $O_2N$ 
 $O_2N$ 
 $O_2N$ 
 $O_3N$ 
 $O_4N$ 
 $O_4N$ 
 $O_4N$ 
 $O_5N$ 
 $O_5N$ 

RN 590389-88-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-89-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-thiazolylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590389-90-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(5-fluoro-2-methoxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-92-7 CAPLUS

CN Carbamic acid, [(1R)-1-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)methyl]-2-phenylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 590389-93-8 CAPLUS

CN Carbamic acid, [(1S)-1-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)methyl]-2-phenylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 590389-95-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(2-oxo-2-phenylethyl)-4-thioxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN & H \\ N & N \end{array}$$

RN 590389-97-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(2-hydroxy-6-methoxyphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590389-98-3 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(5-bromo-2-furanyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 590389-99-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[2-(phenylmethoxy)ethyl]-4-thioxo- (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-CH_2-CH_2 \xrightarrow{N} \xrightarrow{N} \stackrel{CN}{\underset{N}{\bigvee}}$$

RN 590390-00-4 CAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)methyl]-2,2-dimethyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 590390-01-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[2-(4-hydroxyphenyl)-2-oxoethyl]-4-thioxo- (9CI) (CA INDEX NAME)

HO O 
$$C-CH_2-N$$
  $N$   $N$   $N$   $N$   $N$   $N$   $N$   $N$ 

RN 590390-02-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[5-(2-chlorophenyl)-2-furanyl]methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590390-03-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[[5-(2-nitrophenyl)-2-furanyl]methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590390-04-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[3-fluoro-4-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$F_3C$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590390-05-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2,2-dimethyl-1,3-dioxolan-4-yl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{O} \end{array} \begin{array}{c} \text{CH}_2 \\ \text{N} \\ \text{S} \end{array}$$

RN 590390-06-0 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

590390-07-1 CAPLUS RN

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(2-hydroxy-5-methylphenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN

590390-08-2 CAPLUS 1H-Pyrrole, 2-[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-CN pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)methyl]-1-(phenylsulfonyl) - (9CI) (CA INDEX NAME)

RN590390-09-3 CAPLUS

CN1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[[2-chloro-3-(trifluoromethyl)phenyl]methyl]-4,6,7,8,9,10-hexahydro-4thioxo- (9CI) (CA INDEX NAME)

$$F_3C$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590390-10-6 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[[1-[(2-nitrophenyl)methyl]-1H-pyrrol-2-yl]methyl]-4-thioxo- (9CI) (CA INDEX NAME)

$$O_2N$$
 $CH_2$ 
 $N$ 
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590390-11-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(5-fluoro-2-hydroxyphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590390-12-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(1H-indol-7-ylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 590390-13-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(1-methyl-1H-imidazol-2-yl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590390-14-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(3-chloro-2-fluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

$$C1$$
 $CH_2$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 590390-15-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(4-fluoro-3-nitrophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590390-16-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[[4-(2-pyridinyl)phenyl]methyl]-4-thioxo- (9CI) (CA INDEX NAME)

RN 590390-17-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(3-cyano-4-fluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 590390-18-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(1-methyl-1H-indol-2-yl)methyl]-4-thioxo- (9CI) (CA INDEX NAME)

RN 590390-19-5 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-[(2-methoxy-5-nitrophenyl)methyl]-4-thioxo-(9CI) (CA INDEX NAME)

RN 590390-20-8 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-ll-carbonitrile, 8-[(4-acetylphenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 590390-21-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-[(2,6-difluorophenyl)methyl]-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
CN & H \\
N & N \\
F & S
\end{array}$$

RN 590390-22-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 10-amino-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 590390-23-1 CAPLUS

CN Benzamide, N-(11-cyano-4,6,7,8,9,10-hexahydro-4-oxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-10-yl)-N-methyl- (9CI) (CA INDEX NAME)

RN 590390-24-2 CAPLUS

CN 8H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-8-carbothioamide, 11-cyano-1,4,6,7,9,10-hexahydro-N-[2-(4-morpholinyl)ethyl]-4-thioxo- (9CI) (CA INDEX NAME)

RN 590390-25-3 CAPLUS

CN Carbamic acid, [[[(11-cyano-1,4,6,7,9,10-hexahydro-4-thioxo-8H-pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepin-8-yl)thioxomethyl]amino]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 590390-26-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(4-nitrophenyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 590390-27-5 CAPLUS

CN Pyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-8-(3-methyl-1-oxobutyl)-4-oxo-(9CI) (CA INDEX NAME)

RN 590390-28-6 CAPLUS

CN Benzamide, N-[1-[(10-cyano-4,6,7,9-tetrahydro-4-oxopyrazino[1',2':1,5]pyrrolo[3,2-d]pyrimidin-8(1H)-yl)carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

IT 590390-36-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of pyrrolopyrimidine derivs. as GSK-3 inhibitors)

RN 590390-36-6 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## 10/505,228

L10 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:396457 CAPLUS

DOCUMENT NUMBER: 138:385446

TITLE: Preparation of 9-deazaguanine derivatives as

inhibitors of GSK-3 and ROCK kinase

INVENTOR(S): Cao, Jingrong; Choquette, Debbie; Davies, Robert;

Forster, Cornelia; Lauffer, David; Pierce, Albert; Tomlinson, Ronald; Wannamaker, Marion; Metz, Natalie

PATENT ASSIGNEE(S):

SOURCE: U.S. Pat. Appl. Publ., 38 pp.

Patent

CODEN: USXXCO

DOCUMENT TYPE:

English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<del>-</del>				
US 2003096813	A1	20030522	US 2002-125885	20020419
PRIORITY APPLN. INFO.:			US 2001-285217P P	20010420
OTHER SOURCE(S):	MARPAT	138:385446	•	

Ι

GI

AB The present invention provides 9-deazaguanine derivs. I [X = 0, S; Y = S,O, NR1; R1 = H, aliphatic, carboxy, acyl, etc.; R2 = H, aliphatic, alkoxy, thioalkoxy, etc; R3 = H, aliphatic, CN, halo, NO, etc.; R4 = H, aliphatic, amino, amido, etc.], e.g., 4-thioxo-3,4,5,6,7,8-hexahydro-1,3,4btriazafluorene-9-carbonitrile. These compds. are inhibitors of protein kinase, particularly inhibitors of GSK-3 mammalian protein kinase. The invention also provides pharmaceutical compns. comprising the inhibitors of the invention and methods of using those compns. in the treatment and prevention of various disorders, such as diabetes and Alzheimer's disease. IC50 and Ki detns. for inhibition of GSK-3 showed that many I have values below one  $\mu M$  and IC50 detns. for ROCK inhibition showed that certain I inhibit ROCK kinase. Although the methods of preparation are not claimed, 39 example prepns. of I are included.

132994-09-3P 136203-44-6P 473996-90-6P, 4-Thioxo-3,4,5,6,7,8-hexahydro-1,3,4b-triazafluorene-9-carbonitrile 473996-91-7P 473996-94-0P 473996-95-1P 473996-98-4P 473996-99-5P 473997-00-1P 473997-01-2P 473997-33-0P 473997-34-1P 473997-46-5P 473997-47-6P 473997-48-7P 473997-49-8P 473997-50-1P 473997-51-2P 473997-52-3P 473997-53-4P 473997-54-5P 473997-55-6P 473997-56-7P 473997-57-8P 473997-58-9P 473997-59-0P 473997-60-3P

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473997-61-4P 473997-62-5P 473997-63-6P
473997-64-7P 473997-65-8P 473997-66-9P
473997-67-0P 473997-68-1P 473997-69-2P
473997-70-5P 473997-71-6P 473997-72-7P
473997-73-8P 473997-74-9P 473997-75-0P
473997-76-1P 473997-77-2P 473997-78-3P
473997-79-4P 473997-80-7P 473997-81-8P
473997-82-9P 473997-83-0P 473997-84-1P
473997-85-2P 473997-86-3P 473997-87-4P
473997-88-5P 473997-89-6P 473997-90-9P
473997-91-0P 473997-92-1P 473997-93-2P
473997-94-3P 473997-95-4P 473997-96-5P
473997-97-6P 473997-98-7P 473997-99-8P
473998-00-4P 473998-01-5P 473998-02-6P
473998-03-7P 473998-04-8P 473998-05-9P
473998-06-0P 473998-24-2P 473998-26-4P
473998-27-5P 473998-29-7P 473998-30-0P
473998-31-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; preparation of 9-deazaguanine derivs. as inhibitors of
   GSK-3 and ROCK kinase)
132994-09-3 CAPLUS
Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-oxo-
      (CA INDEX NAME)
```

RN

CN

RN 136203-44-6 CAPLUS CN 1H-Pyrimido[4,5-b]pyrrolizine-9-carbonitrile, 4,6,7,8-tetrahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 473996-90-6 CAPLUS
CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

10/505,228

RN 473996-91-7 CAPLUS

CN Pyrimido[4',5':4,5]pyrrolo[1,2-a]azocine-12-carbonitrile, 1,4,6,7,8,9,10,11-octahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473996-94-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-(9CI) (CA INDEX NAME)

RN 473996-95-1 CAPLUS

CN 3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-3-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473996-98-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 2-cyclopropyl-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 473996-99-5 CAPLUS

CN Benzamide, N-(11-cyano-4,6,7,8,9,10-hexahydro-4-oxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

RN 473997-00-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide, 4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 473997-01-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-4(6H)-one, 7,8,9,10-tetrahydro-(9CI) (CA INDEX NAME)

## 10/505,228

RN 473997-33-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

RN 473997-34-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-46-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxylic acid, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-47-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-acetonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-48-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-methyl- (9CI) (CA INDEX NAME)

RN 473997-49-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-acetamide, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-50-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-acetic acid, 4,6,7,8,9,10-hexahydro-4-thioxo-, methyl ester (9CI) (CA INDEX NAME)

RN 473997-51-2 CAPLUS CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 11-ethynyl-7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)

RN 473997-52-3 CAPLUS
CN Ethanone, 1-(4,6,7,8,9,10-hexahydro-4-thioxo-1Hpyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)- (9CI) (CA INDEX NAME)

RN 473997-53-4 CAPLUS
CN Ethanone, 1-(4,6,7,8,9,10-hexahydro-4-thioxo-1Hpyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)-, O-methyloxime (9CI) (CA
INDEX NAME)

RN 473997-54-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-propanenitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-55-6 CAPLUS

CN Ethanone, 1-(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)-, methylhydrazone (9CI) (CA INDEX NAME)

RN 473997-56-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 11-(3-aminopropyl)-7,8,9,10-tetrahydro-(9CI) (CA INDEX NAME)

RN 473997-57-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-acetic acid, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-58-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxylic acid, 4,6,7,8,9,10-hexahydro-4-thioxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 473997-59-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-[(methylsulfonyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2 & O \\ \parallel & S - Me \\ \hline \\ N & O \\ \hline \\ S & S \end{array}$$

RN 473997-60-3 CAPLUS

CN Methanesulfonamide, N-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)methyl]- (9CI) (CA INDEX NAME)

RN 473997-61-4 CAPLUS

CN Acetamide, N-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)methyl]- (9CI) (CA INDEX NAME)

RN 473997-62-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

RN 473997-63-6 CAPLUS CN 1-Propanone, 1-(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)- (9CI) (CA INDEX NAME)

RN 473997-66-9 CAPLUS CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,

7,8,9,10-tetrahydro-11-(2H-1,2,3-triazol-4-yl)- (9CI) (CA INDEX NAME)

RN 473997-67-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(5-methyl-1,3,4-oxadiazol-2-yl)- (9CI) (CA INDEX NAME)

RN 473997-68-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(5-methyl-1,3,4-thiadiazol-2-yl)- (9CI) (CA INDEX NAME)

RN 473997-69-2 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(5-methyl-2-thiazolyl)- (9CI) (CA INDEX NAME)

RN 473997-70-5 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(5-methyl-2-oxazolyl)- (9CI) (CA INDEX NAME)

RN 473997-71-6 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
 7,8,9,10-tetrahydro-11-(3-isoxazolyl)- (9CI) (CA INDEX NAME)

RN 473997-73-8 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(1H-pyrazol-1-yl)- (9CI) (CA INDEX NAME)

RN 473997-74-9 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(1-methyl-1H-1,2,4-triazol-3-yl)- (9CI) (CA INDEX NAME)

RN 473997-75-0 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-

1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(3-methyl-1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

RN 473997-76-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(5-isoxazolyl)- (9CI) (CA INDEX NAME)

RN 473997-77-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide, 4,6,7,8,9,10-hexahydro-N-2-thiazolyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-78-3 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide, 4,6,7,8,9,10-hexahydro-N-1H-pyrazol-3-yl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-79-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide, N-(1,1-dimethylethyl)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-80-7 CAPLUS

CN Piperidine, 1-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-

pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 473997-81-8 CAPLUS

CN Morpholine, 4-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 473997-82-9 CAPLUS

CN Thiomorpholine, 4-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 473997-83-0 CAPLUS
CN Piperazine, 1-[(4,6,7,8,9,10-hexahydro-4-thioxo-1Hpyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)carbonyl]-4-methyl- (9CI)
(CA INDEX NAME)

RN 473997-84-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide,
4,6,7,8,9,10-hexahydro-N-(phenylmethyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 473997-85-2 CAPLUS CN Urea, [(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2a]azepin-11-yl)methyl]- (9CI) (CA.INDEX NAME)

RN 473997-86-3 CAPLUS

CN Benzenesulfonamide, N-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-NH-S-Ph \\ \parallel & \parallel \\ N & \parallel \\ N & \parallel \\ N & \parallel \\ S & \parallel \end{array}$$

RN 473997-87-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 10-amino-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-88-5 CAPLUS

CN Acetamide, N-(11-cyano-4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-10-yl)- (9CI) (CA INDEX NAME)

10/505,228

RN 473997-89-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 9-amino-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-90-9 CAPLUS

CN Acetamide, N-(11-cyano-4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-9-yl)- (9CI) (CA INDEX NAME)

RN 473997-91-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-10-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-92-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,

4,6,7,8,9,10-hexahydro-9-methoxy-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-93-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-9,10-dimethyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-94-3 CAPLUS

CN Carbamic acid, (11-cyano-4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-9-yl)-, methyl ester (9CI) (CA INDEX NAME)

RN 473997-95-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 9-(dimethylamino)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-96-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 473997-97-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-2-propyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-98-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-2-phenyl-4-thioxo-(9CI) (CA INDEX NAME)

RN 473997-99-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-2-(1-methylethyl)-4-thioxo-(9CI) (CA INDEX NAME)

RN 473998-00-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 2-amino-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-01-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-2-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-02-6 CAPLUS

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-thioxo-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 473998-03-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,

4,6,7,8,9,10-hexahydro-2-(phenylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-04-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxylic acid, 4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 473998-05-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 11-amino-7,8,9,10-tetrahydro-(9CI) (CA INDEX NAME)

RN 473998-06-0 CAPLUS

CN Acetamide, N-(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)- (9CI) (CA INDEX NAME)

## 10/505,228

RN 473998-24-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-26-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-27-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-acetyl-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-29-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-30-0 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-a][1,4]diazepine-ll-carbonitrile, 4,6,7,8,9,10-hexahydro-9-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-31-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(phenylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

IT 132994-10-6 178307-15-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 9-deazaguanine derivs. as inhibitors of GSK-3 and ROCK
 kinase)

RN 132994-10-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 178307-15-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

IT 473996-93-9P 473996-96-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 9-deazaguanine derivs. as inhibitors of GSK-3 and ROCK kinase)

RN 473996-93-9 CAPLUS

CN Pyrimido[4',5':4,5]pyrrolo[1,2-a]azocine-12-carbonitrile, 1,4,6,7,8,9,10,11-octahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 473996-96-2 CAPLUS

CN 3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)

L10 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:832804 CAPLUS

DOCUMENT NUMBER: 137:337910

TITLE: Preparation of 9-deazaguanine derivatives as

inhibitors of GSK-3 and ROCK kinase

INVENTOR(S): Cao, Jingrong; Choquette, Debbie; Davies, Robert;

> Forster, Cornelia; Lauffer, David; Pierce, Albert; Tomlinson, Ronald; Wannamaker, Marion; Metz, Natalie

PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 106 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.					KIND		DATE		APPLICATION NO.					DATE			
					A1		20021031		WO 2002-US12395						20020419		
WO	2002085909			A8													
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		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
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		ŬΑ,	ŪĠ,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW			-			-	
	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,
								ΑT,									
		GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,
		GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG							
AU	AU 2002305205				A1 20021105				AU 2002-305205						20020419		
CA	CA 2444598				A1 20031031				CA 2002-2444598						20020419		
EP	EP 1383771				A1 2004012			0128	EP 2002-734012						20020419		
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PRIORITY APPLN. INFO.:						-		1	US 2	001-	2852	17P	]	P 2	0010	420	
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OTHER SOURCE(S): GI					MAR:	PAT	137:	3379:	10								

Ι

AΒ The present invention provides 9-deazaguanine derivs. (shown as I; e.g. 4-thioxo-3,4,5,6,7,8-hexahydro-1,3,4b-triazafluorene-9-carbonitrile) or a pharmaceutically acceptable derivative thereof, wherein X is O or S; Y is -S-, IT

-O- or -NR1-; and R2, R3, and R4 are as described in the specification. These compds. are inhibitors of protein kinase, particularly inhibitors of GSK-3 mammalian protein kinase. The invention also provides pharmaceutical compns. comprising the inhibitors of the invention and methods of using those compns. in the treatment and prevention of various disorders, such as diabetes and Alzheimer's disease. IC50 and Ki detns. for inhibition of GSK-3 showed that many I have values below one  $\mu M$  and IC50 detns. for ROCK inhibition showed that certain I inhibit ROCK kinase. Although the methods of preparation are not claimed, 39 example prepns. of I are included. 132994-09-3P 136203-44-6P 473996-90-6P,

4-Thioxo-3,4,5,6,7,8-hexahydro-1,3,4b-triazafluorene-9-carbonitrile 473996-91-7P 473996-94-0P 473996-95-1P 473996-98-4P 473996-99-5P 473997-00-1P 473997-01-2P 473997-33-0P 473997-34-1P 473997-46-5P 473997-47-6P 473997-48-7P 473997-49-8P 473997-50-1P 473997-51-2P 473997-52-3P 473997-53-4P 473997-54-5P 473997-55-6P 473997-56-7P 473997-57-8P 473997-58-9P 473997-59-0P 473997-60-3P 473997-61-4P 473997-62-5P 473997-63-6P 473997-64-7P 473997-65-8P 473997-66-9P 473997-67-0P 473997-68-1P 473997-69-2P 473997-70-5P 473997-71-6P 473997-72-7P 473997-73-8P 473997-74-9P 473997-75-0P 473997-76-1P 473997-77-2P 473997-78-3P 473997-79-4P 473997-80-7P 473997-81-8P 473997-82-9P 473997-83-0P 473997-84-1P 473997-85-2P 473997-86-3P 473997-87-4P 473997-88-5P 473997-89-6P 473997-90-9P 473997-91-0P 473997-92-1P 473997-93-2P 473997-94-3P 473997-95-4P 473997-96-5P 473997-97-6P 473997-98-7P 473997-99-8P 473998-00-4P 473998-01-5P 473998-02-6P 473998-03-7P 473998-04-8P 473998-05-9P 473998-06-0P 473998-24-2P 473998-26-4P 473998-27-5P 473998-29-7P 473998-30-0P 473998-31-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of 9-deazaguanine derivs. as inhibitors of GSK-3 and ROCK kinase)

132994-09-3 CAPLUS

Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN

CN

RN 136203-44-6 CAPLUS

CN 1H-Pyrimido[4,5-b]pyrrolizine-9-carbonitrile, 4,6,7,8-tetrahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 473996-90-6 CAPLUS

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 473996-91-7 CAPLUS

CN Pyrimido[4',5':4,5]pyrrolo[1,2-a]azocine-12-carbonitrile, 1,4,6,7,8,9,10,11-octahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473996-94-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)

RN 473996-95-1 CAPLUS

CN 3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-3-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473996-98-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 2-cyclopropyl-4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 473996-99-5 CAPLUS

CN Benzamide, N-(11-cyano-4,6,7,8,9,10-hexahydro-4-oxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

RN 473997-00-1 CAPLUS

.CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide, 4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 473997-01-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-4(6H)-one, 7,8,9,10-tetrahydro-(9CI) (CA INDEX NAME)

RN 473997-33-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

RN 473997-34-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-46-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxylic acid, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-47-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-acetonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-48-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-methyl- (9CI) (CA INDEX NAME)

RN 473997-49-8 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-acetamide,
4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-50-1 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-acetic acid,
4,6,7,8,9,10-hexahydro-4-thioxo-, methyl ester (9CI) (CA INDEX NAME)

RN 473997-51-2 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
11-ethynyl-7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)

RN 473997-52-3 CAPLUS CN Ethanone, 1-(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)- (9CI) (CA INDEX NAME)

RN 473997-53-4 CAPLUS

CN Ethanone, 1-(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)-, O-methyloxime (9CI) (CA INDEX NAME)

RN 473997-54-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-propanenitrile, 4,6,7,8,9,10-hexahydro-4-thioxo-(9CI) (CA INDEX NAME)

RN 473997-55-6 CAPLUS

CN Ethanone, 1-(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)-, methylhydrazone (9CI) (CA INDEX NAME)

RN 473997-56-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 11-(3-aminopropyl)-7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)

RN 473997-57-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-acetic acid, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-58-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxylic acid, 4,6,7,8,9,10-hexahydro-4-thioxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 473997-59-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-[(methylsulfonyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{CH}_2 & & & \\ & &$$

RN 473997-60-3 CAPLUS

CN Methanesulfonamide, N-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \circ \\ \parallel & \cdots & \parallel \\ \text{CH}_2 - \text{NH} - \text{S} - \text{Me} \\ \parallel & \parallel & \circ \\ N & \cdots & N \\ \hline & N & \cdots & N \\ \end{array}$$

RN 473997-61-4 CAPLUS

CN Acetamide, N-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)methyl]- (9CI) (CA INDEX NAME)

RN 473997-62-5 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

RN 473997-63-6 CAPLUS CN 1-Propanone, 1-(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)- (9CI) (CA INDEX NAME)

RN 473997-64-7 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(5-methyl-1,2,4-oxadiazol-3-yl)- (9CI) (CA INDEX NAME)

RN 473997-65-8 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(3-methyl-1,2,4-oxadiazol-5-yl)- (9CI) (CA INDEX

NAME)

RN 473997-66-9 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(2H-1,2,3-triazol-4-yl)- (9CI) (CA INDEX NAME)

RN 473997-67-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(5-methyl-1,3,4-oxadiazol-2-yl)- (9CI) (CA INDEX NAME)

RN 473997-68-1 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(5-methyl-1,3,4-thiadiazol-2-yl)-(9CI) (CA INDEX NAME)

RN 473997-69-2 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(5-methyl-2-thiazolyl)- (9CI) (CA INDEX NAME)

RN 473997-70-5 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione,
7,8,9,10-tetrahydro-11-(5-methyl-2-oxazolyl)- (9CI) (CA INDEX NAME)

## 10/505,228

RN 473997-71-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(3-isoxazolyl)- (9CI) (CA INDEX NAME)

RN 473997-72-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(2H-tetrazol-2-yl)- (9CI) (CA INDEX NAME)

RN 473997-73-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(1H-pyrazol-1-yl)- (9CI) (CA INDEX NAME)

RN 473997-74-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(1-methyl-1H-1,2,4-triazol-3-yl)- (9CI) (CA INDEX NAME)

RN 473997-75-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(3-methyl-1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)

RN 473997-76-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 7,8,9,10-tetrahydro-11-(5-isoxazolyl)- (9CI) (CA INDEX NAME)

RN 473997-77-2 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide,
4,6,7,8,9,10-hexahydro-N-2-thiazolyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-78-3 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide,
4,6,7,8,9,10-hexahydro-N-1H-pyrazol-3-yl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-79-4 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide,
N-(1,1-dimethylethyl)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-80-7 CAPLUS

CN Piperidine, 1-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 473997-81-8 CAPLUS

CN Morpholine, 4-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 473997-82-9 CAPLUS

CN Thiomorpholine, 4-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-

pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-ll-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 473997-83-0 CAPLUS

CN Piperazine, 1-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 473997-84-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxamide, 4,6,7,8,9,10-hexahydro-N-(phenylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-85-2 CAPLUS

CN Urea, [(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)methyl]- (9CI) (CA INDEX NAME)

RN 473997-86-3 CAPLUS

CN Benzenesulfonamide, N-[(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)methyl]- (9CI) (CA INDEX NAME)

RN 473997-87-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 10-amino-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-88-5 CAPLUS

CN Acetamide, N-(11-cyano-4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-10-yl)- (9CI) (CA INDEX NAME)

RN 473997-89-6 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,
9-amino-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-90-9 CAPLUS
CN Acetamide, N-(11-cyano-4,6,7,8,9,10-hexahydro-4-thioxo-1Hpyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-9-yl)- (9CI) (CA INDEX NAME)

RN 473997-91-0 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-10-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-92-1 CAPLUS CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,

4,6,7,8,9,10-hexahydro-9-methoxy-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-93-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-9,10-dimethyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-94-3 CAPLUS

CN Carbamic acid, (11-cyano-4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-9-yl)-, methyl ester (9CI) (CA INDEX NAME)

RN 473997-95-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 9-(dimethylamino)-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-96-5 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-4-thioxo-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 473997-97-6 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-2-propyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-98-7 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-2-phenyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473997-99-8 CAPLUS
CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,
4,6,7,8,9,10-hexahydro-2-(1-methylethyl)-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-00-4 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 2-amino-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-01-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-2-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-02-6 CAPLUS

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-thioxo-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 473998-03-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile,

4,6,7,8,9,10-hexahydro-2-(phenylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

$$CN$$
 $H$ 
 $N$ 
 $CH_2-Ph$ 
 $S$ 

RN 473998-04-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carboxylic acid, 4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 473998-05-9 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-4(6H)-thione, 11-amino-7,8,9,10-tetrahydro- (9CI) (CA INDEX NAME)

RN 473998-06-0 CAPLUS

CN Acetamide, N-(4,6,7,8,9,10-hexahydro-4-thioxo-1H-pyrimido[4',5':4,5]pyrrolo[1,2-a]azepin-11-yl)- (9CI) (CA INDEX NAME)

RN 473998-24-2 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-26-4 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-27-5 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 8-acetyl-4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-29-7 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-30-0 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-9-methyl-4-thioxo- (9CI) (CA INDEX NAME)

RN 473998-31-1 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-d][1,4]diazepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-8-(phenylmethyl)-4-thioxo- (9CI) (CA INDEX NAME)

IT 132994-10-6 178307-15-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 9-deazaguanine derivs. as inhibitors of GSK-3 and ROCK kinase)

RN 132994-10-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 178307-15-8 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

IT 473996-93-9P 473996-96-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 9-deazaguanine derivs. as inhibitors of GSK-3 and ROCK kinase)

RN 473996-93-9 CAPLUS

CN Pyrimido[4',5':4,5]pyrrolo[1,2-a]azocine-12-carbonitrile, 1,4,6,7,8,9,10,11-octahydro-4-oxo- (9CI) (CA INDEX NAME)

RN 473996-96-2 CAPLUS

CN 3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-3-methyl-4-oxo- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

LINO ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:434877 CAPLUS

DOCUMENT NUMBER: 125:48517

TITLE: Acetals of acid lactams and amides. 74. Examining the

synthesis and antitumor action of 5,6 polymethylenepyrrolo [3,2-d] pyrimidines

AUTHOR(S): Kadushkin, A. V.; Sokolova, A. S.; Solovyeva, N. P.;

Granik, V. G.

CORPORATE SOURCE: TSKhLS, VNIKhFI, Moscow, Russia

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1994), 28(11),

15-19

CODEN: KHFZAN; ISSN: 0023-1134

PUBLISHER: Meditsina
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Conditions of pyrimidine cyclization as well as roles of ethoxycarbonyl

group and of the polymethylene chain in antitumor activity were studied. IT 178307-15-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (synthesis and antitumor action of polymethylenepyrrolopyrimidines)

RN 178307-15-8 CAPLUS

CN lH-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-ll-carbonitrile, 4,6,7,8,9,10-hexahydro-4-thioxo- (9CI) (CA INDEX NAME)

IT 111038-16-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and antitumor action of polymethylenepyrrolopyrimidines)

RN 111038-16-5 CAPLUS

CN 1H-Pyrimido[4,5-b]pyrrolizine-9-carboxylic acid, 4,6,7,8-tetrahydro-4-thioxo-, ethyl ester (9CI) (CA INDEX NAME)

10 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:559084 CAPLUS

DOCUMENT NUMBER: 115:159084

TITLE: Acetals of lactams and amides. 65. Reaction of DMF

diethyl acetal with derivatives of

6-amino-5-carbamoyl(thiocarbamoyl)pyrrolizine

AUTHOR(S): Kadushkin, A. V.; Solov'eva, N. P.; Golovko, T. V.;

Granik, V. G.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow,

119021, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1991), (3),

349-54

CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE:

Journal Russian

LANGUAGE:

GI

$$R$$
 $NH_2$ 
 $CXR^1$ 
 $I$ 
 $X$ 
 $III$ 

AB The condensation of Me2NCH(OEt)2 with (thio)carbamoylaminopyrrolizines I (R = CN, CO2Et; X = O, S; R1 = NH2) gives aminomethylene derivs. I [R1 = N:CHNMe2 (II)]. On treatment with AcOH II undergo a cyclization to give pyrimidopyrrolizine derivs. III.

IT 111038-16-5P 136203-44-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 111038-16-5 CAPLUS

CN 1H-Pyrimido[4,5-b]pyrrolizine-9-carboxylic acid, 4,6,7,8-tetrahydro-4-thioxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 136203-44-6 CAPLUS

CN 1H-Pyrimido[4,5-b]pyrrolizine-9-carbonitrile, 4,6,7,8-tetrahydro-4-thioxo-(9CI) (CA INDEX NAME)

**⊾**√0 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1991:164140 CAPLUS

DOCUMENT NUMBER:

114:164140

TITLE:

Condensed pyrrolo[3,2-d]pyrimidines: synthesis and

biological activity

AUTHOR(S):

Kadushkin, A. V.; Nesterova, I. N.; Golovko, T. V.;

Nikolaeva, I. S.; Pushkina, T. V.; Fomina, A. N.;

Sokolova, A. S.; Chernov, V. A.; Granik, V. G.

CORPORATE SOURCE:

SOURCE:

VNIKhFI, Moscow, USSR

Khimiko-Farmatsevticheskii Zhurnal (1990), 24(12),

18-22

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE:

LANGUAGE:

Journal Russian

GΙ

$$NH_2$$
 $CO_2$ Et I  $NH_2$ 
 $CN$ 
 $NR$ 
 $NR$ 
 $NR$ 

AB Intramol. Thorpe-Ziegler cyclization was used to prepare 3-cyano-4-amino-5-(ethoxycarbonyl)-1,2-polymethylene pyrrole derivs., e.g. I (n = 1, 2, 3) which were then used in the synthesis of 5,6-polymethylene derivs. of pyrrolo[3,2-d]pyrimidines, e.g. II (R = H, PhCH2, n = 2, 3). The compds. were tested for virucidal and neoplasm-inhibiting activity.

IT 132994-09-3P 132994-10-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and chlorination of)

RN 132994-09-3 CAPLUS

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 1,4,6,7,8,9-hexahydro-4-oxo-(9CI) (CA INDEX NAME)

RN 132994-10-6 CAPLUS

CN 1H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo- (9CI) (CA INDEX NAME)

IT 132994-11-7P 132994-12-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 132994-11-7 CAPLUS

CN Pyrimido[4,5-b]indolizine-10-carbonitrile, 3,4,6,7,8,9-hexahydro-4-oxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 132994-12-8 CAPLUS

CN 3H-Pyrimido[4',5':4,5]pyrrolo[1,2-a]azepine-11-carbonitrile, 4,6,7,8,9,10-hexahydro-4-oxo-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:590445 CAPLUS

DOCUMENT NUMBER: 107:190445

TITLE: Synthesis and antitumor activity of

5-mercapto-9-ethoxycarbonyl-1,2-dihydro-3H-

pyrimido[5,4-e]pyrrolizine derivatives

AUTHOR(S): Kadushkin, A. V.; Golovko, T. V.; Kalistratov, S. G.;

Sokolova, A. S.; Chernov, V. A.; Granik, V. G.

CORPORATE SOURCE: VNIKhFI, Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1987), 21(5),

545-50

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 107:190445

GT

N-Cyanomethyl-2-[cyano(ethoxycarbonyl)methylene]pyrrolidine, obtained from N-cyanomethyl-2-pyrrolidone di-Et acetal and CNCO2Et was cyclized to the dihydropyrrolizine derivative Condensation of this compound with Me2NCH(OEt)2 gave a dimethylaminomethyleneamino derivative which on treatment with NH4SH gave I. The conversion of I to II (R = H, CO2Et or CO2H) and III is described. A study of the antitumor activity of the compds. in rats showed that I, II and III were nontoxic during i.p. administration. The LD was >500 mg/kg. II (R = H) showed cumulative toxicity; after 3 administrations at 250 mg/kg the animals died. II showed antitumor activity in mice with B-16 melanoma. II (R = CO2Et) also showed activity against carcinoma 755.

IT 111038-16-5P 111070-34-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and antitumor activity of)

RN 111038-16-5 CAPLUS

CN lH-Pyrimido[4,5-b]pyrrolizine-9-carboxylic acid, 4,6,7,8-tetrahydro-4-thioxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 111070-34-9 CAPLUS
CN 1H-Pyrimido[4,5-b]pyrrolizine-9-carboxylic acid, 4,6,7,8-tetrahydro-4-oxo-(9CI) (CA INDEX NAME)

ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

CESSION NUMBER: 1981:47260 CAPLUS

DOCUMENT NUMBER: 94:47260

TITLE: Study of lactams. 34. Synthesis and reactions of

pyrrolo[2,3-c]azepine derivatives

AUTHOR(S): Glushkov, R. G.; Stezhko, T. V.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1980), (8),

1097-100

CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE:

Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 94:47260

GI

AB Treatment of hydroxynitrile I (R = OH) with H2NCH2CO2Et gave 60% I (R =NHCH2CO2Et), which was cyclized with EtONa to give 75% II (X = H2), which was treated with Me2NCH(OEt)2 to give 90% II (X = CHNMe2). II (X = H2) was cyclized with HCONH2 to give 98% III (R = R1 = R2 = H). II (X = R1 = R2 = H). CHNMe2) was cyclized with PhCH2NH2 to give 72% III (R = benzyl, R1 = R2 = H), which when treated with Me2NCH2CH2Cl gave 95% III (R = benzyl, Rl =Me2NCH2CH2, R2 = H) (IV). III (R = R1 = R2 = benzyl) was also prepared Cyclization of IV with POC13 gave 42% V.

IT 76237-21-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN76237-21-3 CAPLUS

CN 3,4,8,10,11b-Pentaazacyclohepta[jk]fluoren-11(10H)-one, 1,2,3,5,6,7-hexahydro-3-methyl-10-(phenylmethyl)- (9CI) (CA INDEX NAME)